User's Guide for CEMC_SFU_AGRO v1.2

The Combined Canadian Environmental Modelling Centre Water Quality Model and the Simon Fraser University Food Web Model

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Introduction

The Canadian Environmental Modelling Centre's AGRO modeling system (AGRO) is a MicroSoft Excel® based application that combines a water quality model with a food web model to estimate risk to aquatic species from pesticide exposure in a user-defined water body. A major feature of this system is its capability to incorporate dynamic functionalities which allow the user to introduce changing environmental and emission conditions so that the fate and bioaccumulation results of numerous chemicals can easily and efficiently be compared.

The AGRO modeling system is written in Visual Basic and has an EXCEL® interface for parameter input and output display. This system can be run in dynamic mode which uses daily input of water, sediment, and pesticide from predicted daily mass loadings generated by US EPA Pesticide Root Zone Model, version 3.12 (PRZM3.12) (Suárez, 2006). [Note: AGRO can also be run in a steady-state mode]. Daily loading and emission values from PRZM3.12 are then used to generate predicted daily pesticide concentrations in the water column, benthic pore water and benthic sediment of the water body. From these concentrations, the food web model estimates bioaccumulation of pesticide in aquatic organisms.

The water quality model component of the AGRO modeling system is the Quantitative Water, Air, Sediment Interaction (QWASI) Fugacity model developed by Mackay et al. at the Canadian Environmental Modelling Centre (Mackay, Joy and Paterson (1983), Mackay, Paterson and Joy (1983), Mackay and Diamond (1989), Webster, Lian and Mackay (2005)). The QWASI model is based on a single receiving water body of user-defined size and depth with an active sediment layer. This model can be run in dynamic mode which involves daily input of water from field runoff, dissolved pesticide in field runoff, eroded sediment, pesticide sorbed to eroded sediment, pesticide emissions resulting from application drift and rainfall. These dynamic daily inputs are generated outside of the AGRO modeling system using the EPA PRZM3.12. The AGRO modeling system has built-in capability to import annual mass loading files output from PRZM3.12 and convert these values into the units and configurations needed by the QWASI Fugacity model.

The food web model in AGRO is based on the Bioaccumulation model developed by Frank A.P.C. at Simon Fraser University (Gobas, 2007). The Bioaccumulation model is a dynamic or time dependent interpretation of Arnot and Gobas [2004] bioaccumulation equation. This model is based on the assumption that the exchange of hydrophobic organic chemicals between the organism and its ambient environment can be described by a single equation for a large number of aquatic organisms. For each aquatic organism, this equation estimates bioaccumulation as a function of intake of pesticide via respiration and ingestion of prey, and outflow of pesticide via excretion, metabolism to a daughter product and respiratory exhalation.

System Requirements

The AGRO modeling system is designed to run using MicroSoft Excel® 2003 with at least 10 MB of hard disk space.

Computation Flow Overview

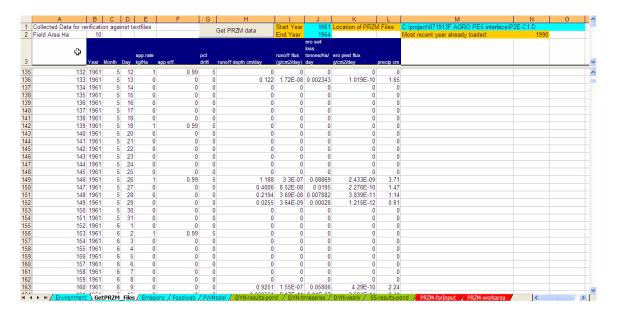
Using Visual Basic for Applications (VBA) as the programming language allows for the AGRO modeling system to function within the framework of EXCEL spreadsheets, thus facilitating the entry and viewing of both the input parameters and the display and analysis of the subsequent output. The following steps detail how to run the AGRO modeling system.

To run the AGRO modeling system in dynamic mode:

Step 1 - Import Daily Mass Loading Data Generated by PRZM3.12 for use in the QWASI model.

Go to the Get PRZM Files Tab

Here is an example of a Get_PRZM_Files page:



Click the "Get PRZM data" button located on cells Get_PRZM_Files!G(1:2)-Get_PRZM_Files!H(1:2). Clicking this executes a Visual Basic macro which

allows the user to choose the location of the PRZM3.12 P2E-c1.D* mass loading files. Click on any of the P2E-C1.D* files and then "Open" to begin the import of the mass loading values and to store them in this tab. This macro also converts the data into the units and variables compatible with the QWASI model. These converted values are stored in the **PRZMforInput tab**.

Table 1 below summarizes the conversion of massing loading values in the P2E-C1.D* files into the values stored in the **PRZMforInput tab.**

Table 1: Summary of daily input values for AGRO model derived from PRZM output

Parameter	Description
Simday	assigned to evaluate and loop through the total number of
	days of data provided by PRZM
Year Month Day	from PRZM
E to Pond kg/y	this is the 5% spray drift from PRZM expressed as kg/y
Inflow-W Conc	from PRZM expressed in ng/L
ng/L	
Inflow-P Conc	from PRZM expressed in ng/L
ng/L	
Bulk Inflow Conc	uses Inflow-W Conc and Inflow-P Conc with the respective
ng/L	volume fractions to calculate a bulk water concentration of
	chemical
Water Inflow rate	Standard rate defined on Environment worksheet + PRZM
m3/h	runoff
Particulate Inflow	Standard rate derived from Environment worksheet +PRZM
rate m3/h	erosion rate
Inflow-P	derived Inflow and Particulate inflow rates
concentration	
VF-W Inflow	Volume Fraction of water in the inflow
VF-P Inflow	Volume Fraction of particulate in the inflow
rain rate m³/h	converted from cm/day in PRZM to m3/h

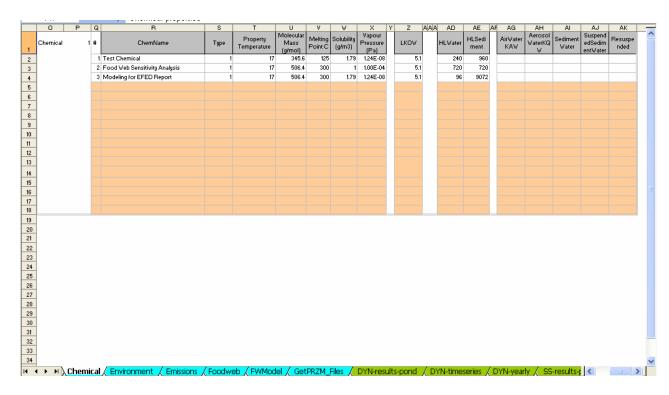
The AGRO modeling system also contains a blank worksheet with tab entitled, **PRZM-workarea**. This worksheet is used by the AGRO Visual Basic module to store internal variable values during processing. It is always cleared at the end of each instance of retrieval of PRZM files.

Step 2 – Enter or Select Chemical Input Parameters

Go to the Chemical tab

The chemical parameters are defined here. A "database" of chemical parameters is listed in columns Chemical!Q through Chemical!AK.

Here is an example of columns Chemical!Q through Chemical!AK in the **Chemical** Tab:



More chemicals can be added to this database or existing chemicals can be modified by entering data into the appropriate columns in the "tan" shaded areas. The names of the newly added chemicals will appear in the list-box entitled "Select a Chemical" in columns Chemical!D-Chemical!F of this tab.

To enter a new chemical with Type I partitioning into the chemical database, enter the following chemical information into the first available empty row:

Table 2: Chemical Parameters for Type I Partitioning Simulations

Column	Parameter	Units	Notes
Chemical!Q	Chemical		The row number plus 1. This
	Identifier		will be used as the chemical
			number identifier.
Chemical!R	Chemical		Name of chemical of interest
	Name		
Chemical!S	Chemical Type		1 for Type I partitioning and 2
			for Type II partitioning. For
			regulatory modeling, Type I
			partitioning is employed.
Chemical!T	Property	°C	Default 17°C
	Temperature		
Chemical!U	Chemical	g/mol	Molecular weight of chemical
	Molecular		
	Mass		
Chemical!V	Chemical	°C	
	Melting Point		
	0		
Chemical!W	Solubility	g/m ³	Water solubility of chemical.
			Equivalent units are kg/L.
Chemical!X	Chemical	Pa	
	Vapor Pressure		
Chemical!Z	Log K _{OW}	(mg/L)/(mg/L)	Log 10 of the Octanol-Water
			Partition Coefficient, K _{OW}
Chemical!AD	Chemical	days	Aqueous aerobic half-life
	Half-life in		
	Water		
Chemical!AE	Chemical	days	Aqueous anaerobic half-life
	Half-life in		
	Sediment		

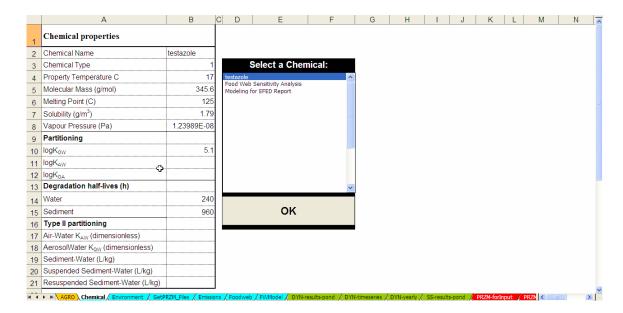
For Type I chemicals, Columns Chemical!AG-Chemical!AK are left blank. For Type II chemicals (those with little or no volatility) only the Molar Mass, Property Temperature, Degradation Half-lives and partition coefficients defined in Chemical!AG:Chemical!AK (with appropriate units) are used. Please see Mackay (2001) for more information on modelling Type I and Type II chemicals.

Table 3: Chemical Parameters for Type I Partitioning Simulations

Column	Parameter	Units	Notes
Chemical!Q	Chemical		The row number plus 1. This
	Identifier		will be used as the chemical
			number identifier.
Chemical!R	Chemical		Name of chemical of interest
	Name		
Chemical!S	Chemical Type		1 for Type I partitioning and 2
			for Type II partitioning.
Chemical!T	Property	°C	Default 17°C
	Temperature		
Chemical!U	Chemical	g/mol	Molecular weight of chemical
	Molecular		
	Mass		
Chemical!AD	Chemical	days	Aqueous aerobic half-life
	Half-life in		
	Water		
Chemical!AE	Chemical	days	Aqueous anaerobic half-life
	Half-life in		
	Sediment		
Chemical!AG	Air/Water	dimensionless	
	Partition		
	Coefficient,		
	K_{AW}		
Chemical!AH	AerosolWater	dimensionless	
	K_{QW}		
Chemical!AI	Sediment-	L/kg	
Chemical:Al	Water	L/Kg	
Chemical!AJ	Suspended	L/kg	
Chemical:AJ	Sediment-Water	y	
Chemical!AK	Resuspended	L/kg	
	Sediment-Water		

Now, go to the list-box "Select a Chemical" in columns Chemical!D-Chemical!F. Highlight the chemical of interest and click the "OK" button. This will cause the appropriate values of the selected chemical to appear in column Chemical!B where the user can easily review them and where the model actually reads the values used in the upcoming simulation. (If the user wishes to make temporary changes to a chemical data, these can be made directly in column Chemical!B without affecting the original values in the database, although these value will be overwritten each time the "OK" button is clicked)

Here is an example of columns Chemical! A through Chemical! N (Rows 1-21) in the **Chemical** tab:



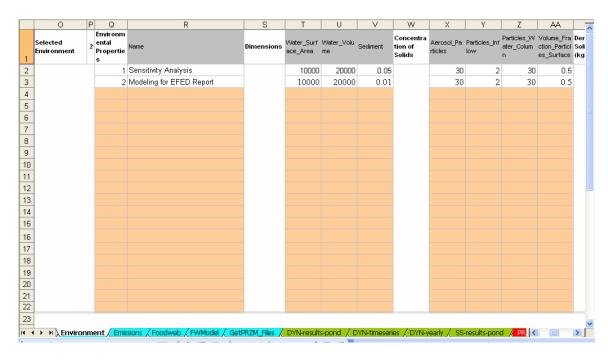
Step 3 – Enter or Select Environment Input Parameters

Go to the **Environment** tab

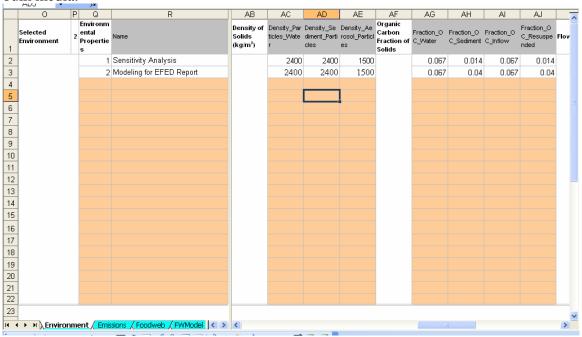
The environment scenario parameters are defined here. A "database" of environmental scenarios is listed in columns Environment!O through Environment!AW. The environmental parameters listed here are those required to run the QWASI 3.10 model.

The user may add environmental scenarios to this database by entering necessary information into the columns Environment!O through Environment!AW. The names of the newly added environments will appear in the list-box entitled "Select an Environment" in this tab.

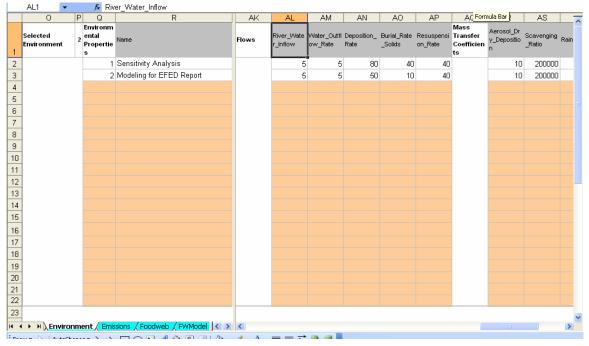
Here is an example of columns Chemical!O through Chemical!AA of the environmental database in the **Environment** tab. Columns Environment!S through Environment!V refer to dimensions of the water body. Columns Environment!W through Environment!AA refer to the concentration of particle solids in the various bulk media. The "tan" cells indicate that the user may input data in these cells.



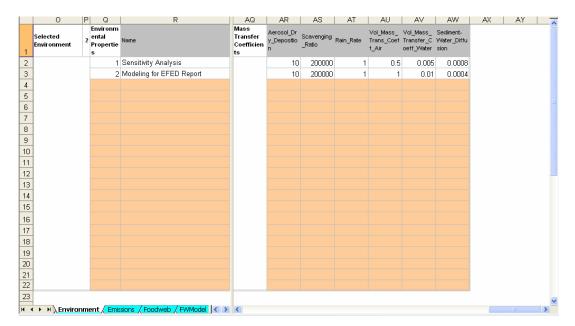
Splitting the screen after column Environment!R and scrolling right, displays columns Environment!AB through Environment!AE which pertain to the density of solids in the various bulk media. Columns Environment!AF through Environment!AJ which pertain to the fraction of organic carbon in the various bulk media.



Splitting the screen after column Environment!R and further scrolling right, displays columns Environment!AK through Environment!AP which pertain to the flow rates for the water and sediment in various bulk media.



Splitting the screen after column Environment!R and further scrolling right, displays columns Environment!AQ through Environment!AW which pertain to the mass transfer coefficients characterizing intermedia transport .



Here is a summary of the input Parameters in the **Environment** Tab:

Table 4: Input Parameters in the Environment Tab

Note: Default values for EPA generic pond scenario are listed in notes column.

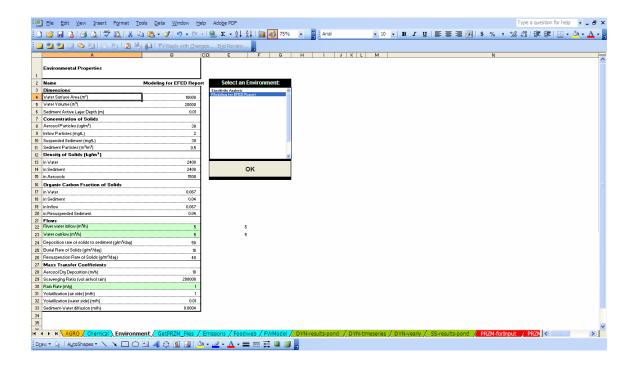
Column	Parameter	Units	Notes				
Environment!O	"Dimensions"		Label for columns associated with				
			dimensions of the water body				
Environment!P	Selected		Numeric identifier of				
	Environment		environmental scenario				
	Identifier		highlighted in the "Select an				
			Environment" list-box.				
			Automatically changes with				
			change in highlighted selection.				
Environment!Q	Environmental		User-supplied numeric identifier				
	Properties		of environmental scenario of				
	Scenario		interest				
	Identifier						
Environment!R	Name of		Name given to the environmental				
	Environmental		scenario				
	Scenario						
Environment!T	Water_Surface_	m^2	Surface area of water body				
	Area	2	Default value: 10,000				
Environment!U	Water_Volume	m ³	Volume of water body				
			Default value: 20,000				
Environment!V	Sediment	m	Depth of sediment in benthic				
			layer.				
			Default value: 0.05				
Environment!W	"Concentration		Label for columns associated with				
	of Solids"		concentration of solid particles in				
		. 3	various bulk media				
Environment!X	Aerosol_Particles	ug/m ³	Concentration of solid particles in				
			air bulk media.				
- AT.	D	77	Default value: 30				
Environment!Y	Particles_Inflow	mg/L	Concentration of solid particles in				
			inflow water bulk media.				
T 1	D 11 111	77	Default Value: 2				
Environment!Z	Particles_Water_	mg/L	Concentration of suspended				
	Column		sediment in water column.				
T	77.1	3, 3	Default value: 30				
Environment!AA	Volume_Fraction	m^3/m^3	Volume fraction of sediment				
	Particles		particles in benthic.				
	Surface		Default value: 0.5				

Column	Parameter	Units	Notes
Environment!AB	"Density of		Label for columns associated with
	Solids"		density of solid particles in
			various bulk media
Environment!AC	Density_Particles	kg/m ³	Density of solid particles in water
	_Water		column bulk media.
			Default value: 2400
Environment!AD	Density_	kg/m ³	Density of solid particles in
	Sediment_		benthic sediment bulk media.
	Particles		Default value: 2400
Environment!AE	Density_Aerosol_	kg/m ³	Density of solids particles in air
	Particles		bulk media.
			Default value: 1500
Environment!AF	"Organic		Label for columns associated with
	Carbon Fraction		organic carbon fraction in various
	of Solids''		bulk media
Environment!AG	Fraction_OC_		Fraction of organic carbon in
	Water		water column bulk media.
			Default value: 0.067
Environment!AH	Fraction_OC_		Fraction of organic carbon in
	Sediment		benthic sediment bulk media
			Default value: 0.014
Environment!AI	Fraction_OC_		Fraction of organic carbon in
	Inflow		inflow water bulk media
			Default value: 0.067
Environment!AJ	Fraction_OC_		Fraction of organic carbon in
	Resuspended		resuspended sediment.
			Default value: 0.014

Column	Parameter	Units	Notes
Environment!AK	"Flows"		Label for columns associated with
			flow rates in various bulk media
Environment!AL	River_Water_	m ³ /h	Flow rate of inflow water into
	Inflow		water body.
			Default value: 5
Environment!AM	Water_Outflow_	m^3/h	Flow rate of outflow water out of
	Rate		the water body.
			Default value: 5
Environment!AN	Deposition_Rate	g/m ²	Deposition rate of solid particles
	_		to benthic sediment.
			Default value: 80
Environment!AO	Burial_Rate_	g/m ²	Burial rate of solid particles in
	Solids		benthic sediment.
			Default value: 40
Environment!AP	Resuspension_	g/m ²	Resuspension rate of solid
	Rate		particles out of the benthic and
			back into the water column.
			Default value: 40
	//2.7. The same of		
Environment!AQ	"Mass Transfer		Label for columns associated with
	Coefficients"		Mass transfer Coefficients
			between various bulk media
Environment!AR	Aerosol_Dry_	m/h	Deposition rate of dry particles
	Deposition		out of air into water body.
		77.1	Default value: 10
Environment!AS	Scavenging_Ratio	Volume of	Scavenging Ratio of air to rain
		air/Volum	Default value: 20,000
		e of Rain	
Environment!AT	Rain_Rate	m/year	Rainfall rate in meters per year.
		-	Default value: 1
Environment!AU	Vol_Mass_	m/h	Volatilization rate – air side
	Trans_Coeff_		Default value: 1
	Air		
Environment!AV	Vol_Mass_	m/h	Volatilization rate – water to air
	Transfer_Coeff_		Default value: 0.01
	Water		
Environment!AW	Sediment-Water-	m/h	Diffusion rate between benthic
	Diffusion		sediment and water column.
			Default value: 0.0004

Now, go to the list-box "Select an Environment" in columns Environment!E-Chemical!G. Highlight the environment of interest and click the "OK" button. This will cause the appropriate values of the selected environment to appear in column Environment!B where the user can easily review them and where the model actually reads the values used in the upcoming simulation. (If the user wishes to make temporary changes to a chemical data, these can be made directly in column Environment!B without affecting the original values in the database, although these value will be overwritten each time the "OK" button is clicked)

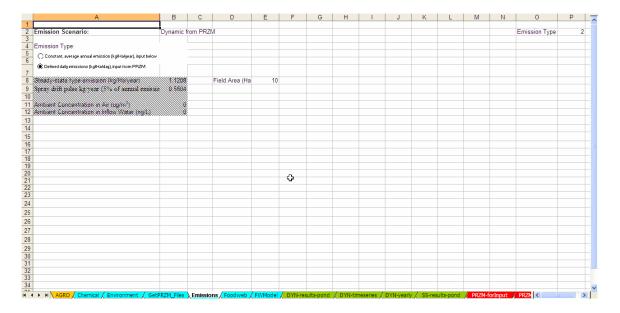
Here is an example of columns Environment! A through Chemical! N (Rows 1-33) in the **Environment** tab:



Step 4 – Confirm the Emissions Parameters

Go to the **Emissions** tab

Here is what the Emissions tab page should look like when dynamic emission scenario is selected:



On the **Emissions tab**, there are two options. By clicking on either radio button under the heading "Emission Type" the user may choose one of two scenarios. The first option is used for steady-state calculations or for dynamic ones requiring that there be constant emission of chemical over the duration of the model run. The second option is to use the PRZM-defined inputs imported to **PRZMforInput** and **GetPRZMFiles tabs**.

Dynamic Emissions

To use the PRZM-defined inputs and parameters, make sure that the "Defined daily emissions (kg/Ha/day), input from PRZM" is selected so that the Emission Type in cell Emissions!P2 is set to 2. Cell Emissions!B2 should say "Dynamic from PRZM" and the cells Emissions!A8:Emissions!E12 appear as though "grayed-out". The above set-up with "Defined daily emissions" selected activates the dynamic mode execution of the model where daily values are read from the **PRZMforInput tab**.

The internal model code automatically navigates through the **PRZMforInput** daily values until it reaches the first non-zero emissions occurrence in PRZMforInput!E column at which time the model iterations begin.

Constant Emissions

If the "Constant Emission, average annual emission (kg/Ha/yr), input below" radio button is selected, the cells Emissions!A8:Emissions!E12 appear with a white background, except cells Emissions!B8, B11 and B12 which are "tan" in colour, indicating that they are user defined inputs. The model reads in the value for calculated direct inputs from spray drift to the pond from cell Emissions!B9. Note that the value of 5% of the application rate to 1 Ha is used to estimate the net input of chemical to the pond from <u>all</u> inputs. This is based on the US-EPA EXAMS model treatment of spray drift inputs to an agricultural pond.

The user may choose to enter any ambient air concentration of chemical in Emissions!B11 or inflow water concentration. Inflow water can be in the form of inflow derived from any source (inflow from another body of water, from groundwater or from runoff water), as long as the corresponding flow for this concentration is quantified on the Environment worksheet. The net annual input of chemical to the pond is derived using:

Conc inflow ng/L * kg/1x10 12 ng * 1000 L/m3 * Inflow rate m3/h * 8760 h/yr

The result (kg/yr) inflow of chemical is added to the kg/yr estimate of direct emission to the pond via spray drift for a total chemical input rate.

Step 5 – Review the FWModel tab

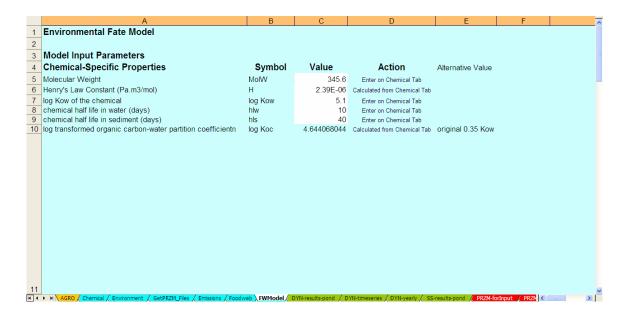
Go to the **FWModel** tab. This tab contains the chemical and ecosystem parameter values used by the Gobas Bioaccumulation model. Review the assigned input values.

Usually, the user will not make any revisions to this tab since the Environmental Fate Parameters on this worksheet are mostly calculated based on values entered in the **Environment and Chemical tabs** and the Food Web Bioaccumulation Model values are the recommended values for the embedded organism foodweb. **Note: There is no database summarizing several possible foodwebs, so any changes made are permanent and it is suggested that an original version of the file be maintained at all times to preserve the original information.**

Columns FWModel!A through FWModel!G summarize the Chemical and Environmental Fate input parameters from the QWASI water quality model.

For columns FWModel!A through FWModel!G, rows 4 - 10, the chemical parameters required by the Bioaccumulation model are automatically summarized based on input values entered in the **Chemical** tab.

An example of columns FWModel!A through FWModel!G, rows 4-10 looks like:



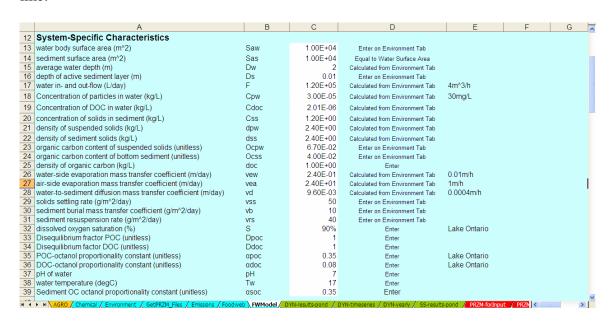
For columns FWModel!A through FWModel!G, rows 12 - 31, the chemical parameters required by the Bioaccumulation model are automatically summarized based on input values entered in the **Environment** tab.

The following additional environmental input parameters along with their recommended values are required by the Bioaccumulation model:

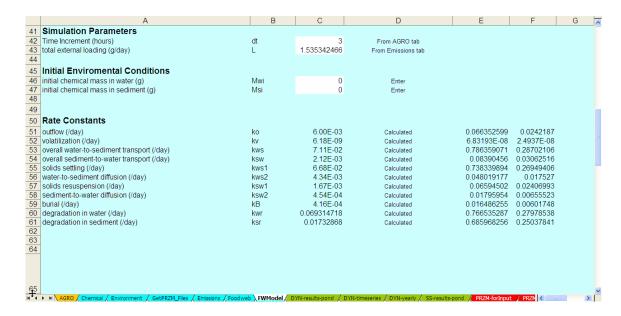
Table 5: Additional Environmental Input parameters in FWModel

Input Parameter	Recommended
	Value
Dissolved oxygen saturation (%)	90%
Disequilibrium factor POC (unitless)	1
Disequilibrium factor DOC (unitless)	1
POC-octanol proportionality constant (unitless)	0.35
DOC-octanol proportionality constant (unitless)	0.08
pH of water	7
water temperature (degC)	17
Sediment OC octanol proportionality constant (unitless)	0.35
initial chemical mass in water (g)	0
initial chemical mass in sediment (g)	0

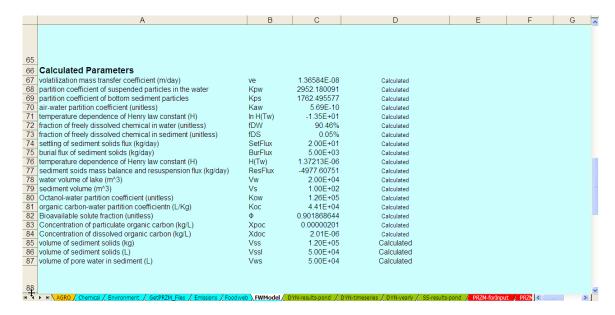
An example of columns FWModel!A through FWModel!G, rows 4-10 looks like:



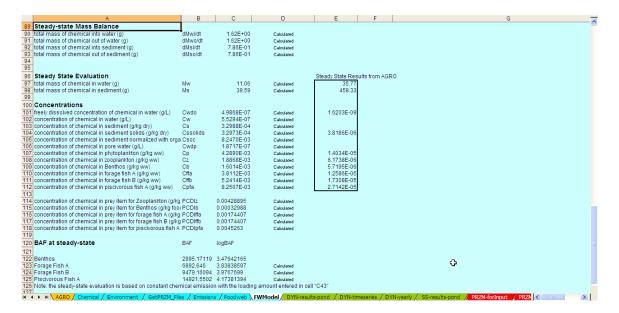
An example of columns FWModel!A through FWModel!G, rows 41 - 65 looks like:



An example of columns FWModel!A through FWModel!G, rows 66 – 87 looks like:

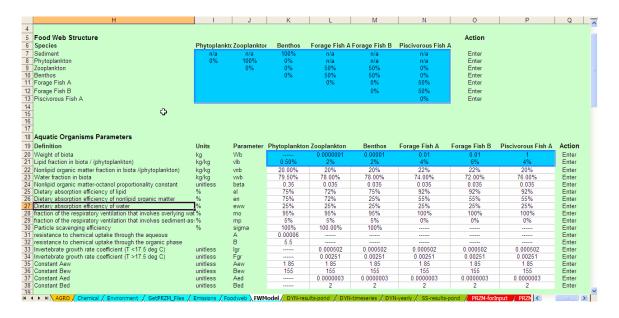


An example of columns FWModel!A through FWModel!G, rows 66 – 87 looks like:

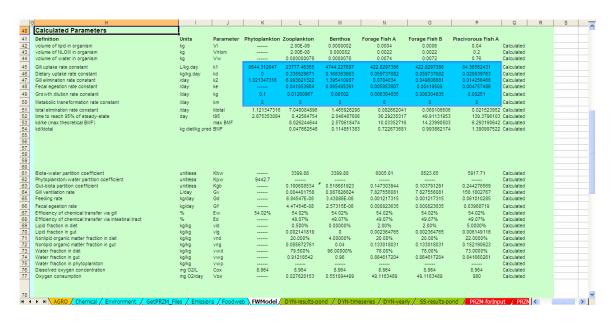


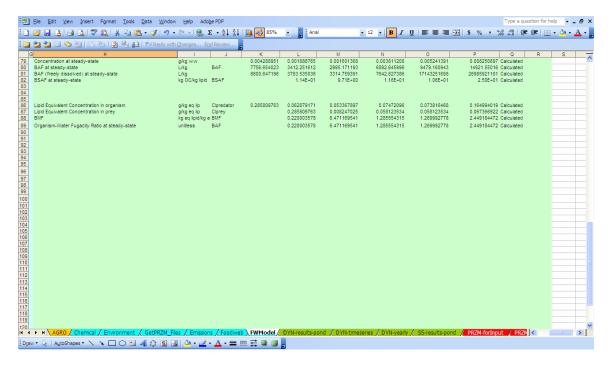
Food Web input values for the Bioaccumulation model are included in columns FWModel!G through FWModel!L.

The food web structure is included in rows 5 through 13. The food web aquatic organism individual parameters are included in rows 18-38. The below page displays the recommended values for these rows:



The calculated parameters for each aquatic organism in the food web are included in rows 40 through 77 and 79-89. The below pages display the recommended values for these rows:



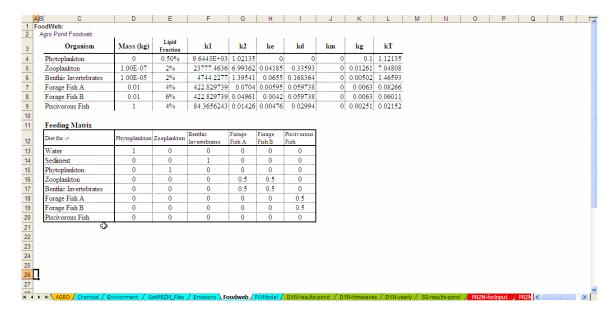


Step 6 – Review the Foodweb tab

Go to the **Foodweb** tab. All values in this tab are automatically summarized from the **FWModel** tab. Thus, the user will never make any revisions to this tab.

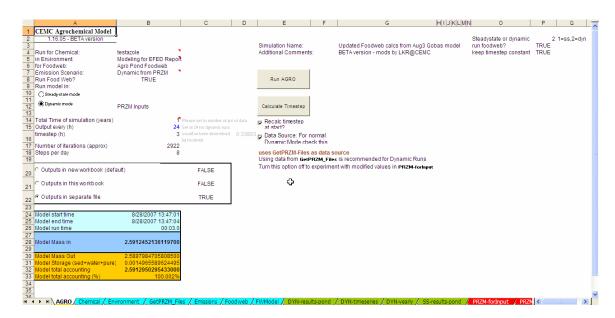
The **Foodweb** tab summarizes the calculated k-values and the Feeding Matrix from the **FWModel tab**. The **Foodweb** tab is where the Bioaccumulation model actually reads in its input values to populate the foodweb and generate organism concentrations.

The page below displays a copy of the **Foodweb tab** with recommended calculated masses, lipid fractions, k-rates, and feeding matrix for the food web.

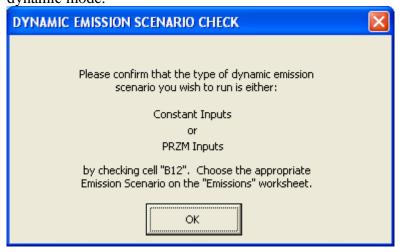


Step 7 – Confirm Run Parameters and Run Simulation

Go to the AGRO tab



Select either dynamic mode or steady-state mode. If Steady-state mode is selected then the emission scenario automatically changes to "Constant Inputs" as defined on the **Emissions tab**. When the dynamic mode is selected a message box appears to remind the user to select the appropriate emissions scenario as the PRZM-based scenario is NOT automatically selected when the model runs in dynamic mode.



Enter the number of years of the simulation in cell AGRO!B14.

To output daily, enter "24" in cell AGRO!B15.

Use the "calculate timestep" button to fill in the appropriate timestep for the modelled system in cell AGRO!B16.

Select the "Outputs in separate file" option.

Cell AGRO!P2 will read 1 if steady-state mode is selected or 2 if dynamic mode is selected.

Cell AGRO!P3 should be set to "TRUE" so that the Bioaccumulation model is run in addition to the QWASI water quality model.

Also, cell AGRO!P4 should also be set to "True" so the timestep set as constant for the entire simulation, otherwise the model attempts to recalculate the timestep required at each iteration.

Examine cells AGRO!B4 – AGRO!B8 to make sure that the correct chemical, environmental scenario, foodweb, and dynamic simulation model options are selected.

Click the "Run AGRO" button to run the simulation.

To monitor the progress of a simulation, each simulation day number is displayed on the lower left-hand corner as it is being processed.

Upon completion of a simulation, Cells AGRO!B24 – AGRO!B33 display the model run time and simulation mass balance.

Step 8 – **Examine the output from the simulation**

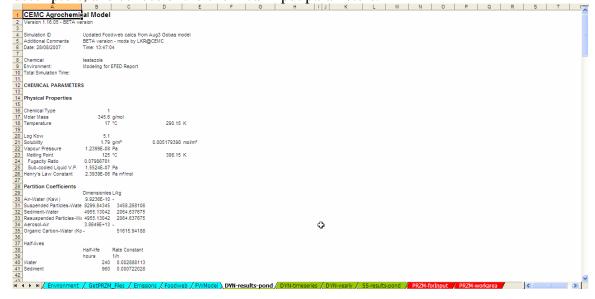
The output from the dynamic mode simulation is displayed in tabs **DYN-results-pond**, **DYN-timeseries**, and **DYN-yearly**. The output from the steady-state mode simulation is displayed in the tab named **SS-results-pond**. An overview of the format of the dynamic results is presented, followed by an overview of the steady-state results.

Dynamic Results

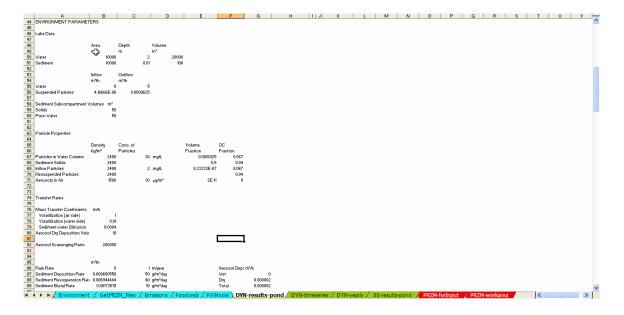
The results presented in the **DYN-results-pond** tab are in the same format as the QWASI model with the foodweb results output at the bottom. These results reflect the **conditions at the end of the simulation**.

The following series of pages display an example of output contained in the **DYN-results-pond** tab.

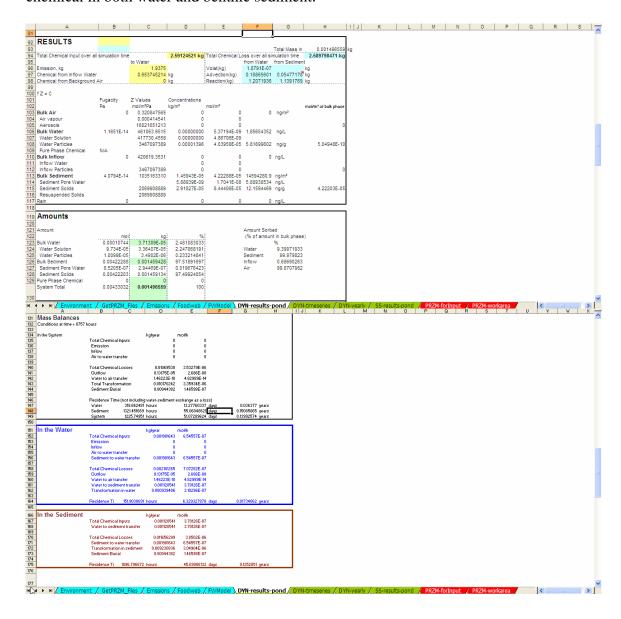
DYN-results-pond tab, Rows 1 - 43 display the model version number, scenario descriptors, and echoes of the chemical input parameters.



DYN-results-pond tab, Rows 44 - 91 display echoes of the environment input parameters.



DYN-results-pond tab, Rows 92 - 228 display results from the QWASI water quality model. These include mass balances over the simulated time for the chemical in both water and benthic sediment.



DYN-results-pond tab, Rows 92 - 228, continued.

11415525.11 11415525.11

32.85109036

72.86729036

4166666667

4166666667

11990.64798

26596.56098

1E+11 1E+11

DYN-results-pond DYN-timeseries DYN-yearly SS-

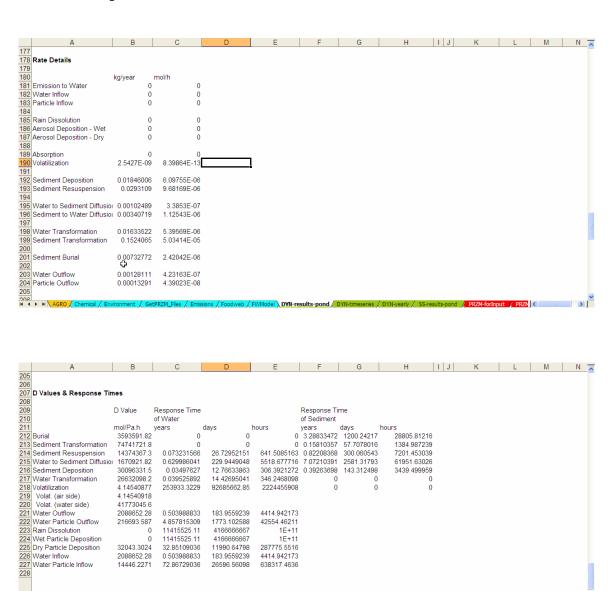
287775 5516

638317.4636

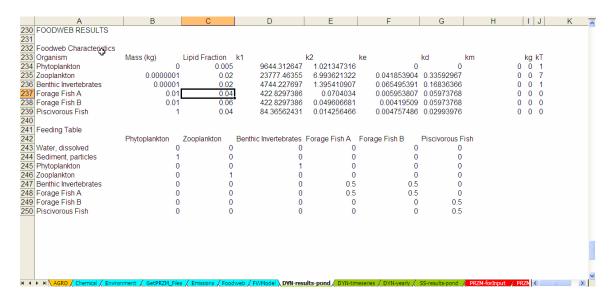
0

32043.3024

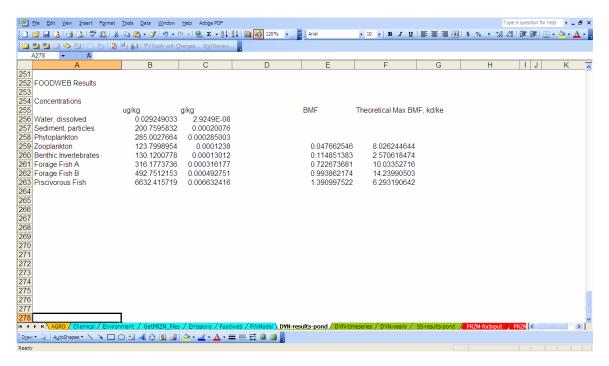
14446.2271



DYN-results-pond tab, Rows 229 - 250 display echoes of the input for the Food Web aquatic organism masses, lip fraction, k-rates and feeding table matrix used by the Bioaccumulation model.

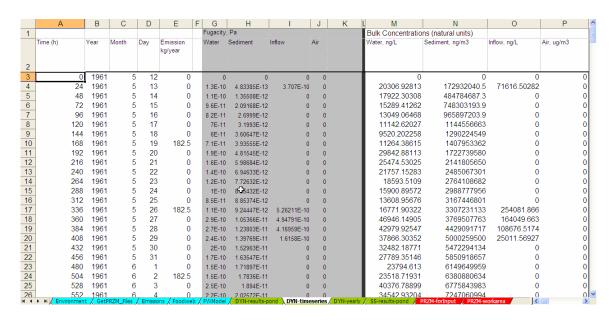


DYN-results-pond tab, Rows 251 - 263 display calculated results of pesticide concentrations from the Bioaccumulation model for each aquatic organism in the food web. The organism Biomagnification Factors (BMFs) and the Theoretical Maximum BMFs (calculated by kd/ke) are presented.

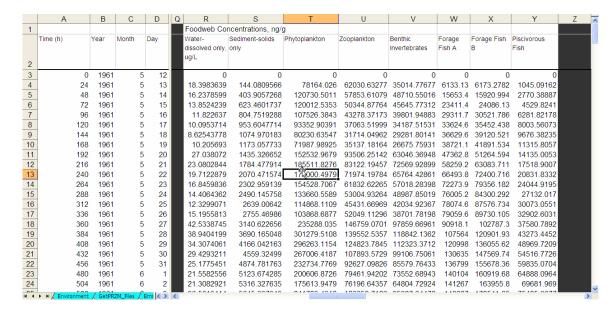


The **DYN-timeseries** tab contains the values of selected output variables for each day of the simulation.

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!P** is displayed below. These columns summarize the daily simulation date, emission, fugacities for each bulk media, and bulk media chemical concentrations in natural units.



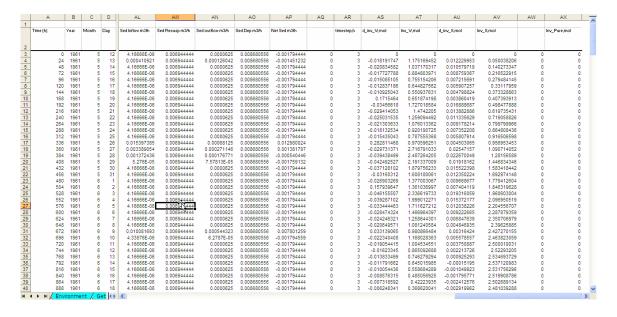
An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!R - DYN-timeseries!Z** is displayed below. These columns summarize the daily chemical concentrations for aquatic organism in the food web.



An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!AA - DYN-timeseries!AJ** is displayed below. These columns display the daily concentrations in the dissolved water column, benthic sediment and pore water along with the total daily input of chemical mass, total daily output of chemical mass, daily water inflow rate, daily water outflow rate, and net daily water volume flux.

	Α	В	С	D	AA	AB	AC	AD	AE	AF	AH AH	Al	AJ	^
1														
2	Time (h)	Year	Month	Day	Water-dissolved only-ug/L-2	Sediment solids only ng/g	Conc porewater ug/L		Suminput, kg	SumLoss, kg	Water inflow m3/h	Water outflow m3/h	Net water m3/h	
3	0	1961	5	12	0	0	0		0	0	5	5		0
4	24	1961	5		18.39836386	0.144080957	0.069785105		0.439666399	0.439666465	10.08333	_		0
5	48	1961	5		16.39636366	0.403905727	0.195630319		0.454831194	0.454831721	10.00333			0
6	72	1961	5		13 8524239	0.403903727			0.454831194	0.454831721	5	5	-	0
7	96	1961	5		11.82263701	0.804751929			0.454831194	0.454831721	5			0
8	120	1961	5		10.09537143	0.953604771			0.454831194	0.454831721	5	5	-	0
9	144	1961	5		8.625437785	1.074970183		,	0.454831194	0.454831721	5			- 1
10	168	1961	5		10.20569304	1.173057733			0.517331194	0.517331721	5	5	Ċ	0
11	192	1961	5		27.03807204	1.435326652	0.695195418		0.954831194	0.954831721	5	5	Ċ	0
12	216	1961	5		23.08028441	1.784477914	0.864305605		0.954831194	0.954831721	5	5	Ċ	0
13	240	1961	5	22	19.71228793	2.070471574	1.002825628		0.954831194	0.954831721	5	5	(0
14	264	1961	5	23	16.84598363	2.302959139	1.115430163		0.954831194	0.954831721	5	5	(0
15	288	1961	5	24	14.40643623	2.490145758	1.206093344		0.954831194	0.954831721	5	5	0	0
16	312	1961	5	25	12.32990715	2.63900642	1.278193482		0.954831194	0.954831721	5	5	(0
17	336	1961	5	26	15.19558134	2.75546986	1.33460214		1.058873579	1.058877616	54.5	54.5	0	0
18	360	1961	5	27	42.53387448	3.140622656	1.521149543		1.797845806	1.797875133	21.69167	21.69167	(0
19	384	1961	5	28	38.94041986	3.690165048	1.787318469		1.87718513	1.877219789	14.14167	14.14167	(0
20	408	1961	5	29	34.30740611	4.166042163	2.017807876		1.909914237	1.909950634	6.0625	6.0625	(0
21	432	1961	5	30	29.4293211	4.55932499	2.208293031		1.913098522	1.913134945	5	5	(0
22	456	1961	5	31	25.17754514	4.874781763	2.36108341		1.913098522	1.913134945	5	5	0	0
23	480	1961	6	1	21.55825564	5.123674285	2.481633628		1.913098522	1.913134945	5	5	0	0
24	504	1961	6	2	21.30829206	5.316327635	2.574944601		1.975598522	1.975634945	5	5	0	0
₩	▶ ► Environment	/ GetPR	ZM_Files 🔏	Emit C	<	F 0.450070.40	0.7040000		0.440000500	0.4404045		_	ĺ	>

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!AL - DYN-timeseries!AX** is displayed below. These columns display the particle solid fluxes in the water column and benthic sediment along with various water and sediment daily fluxes in mol basis.

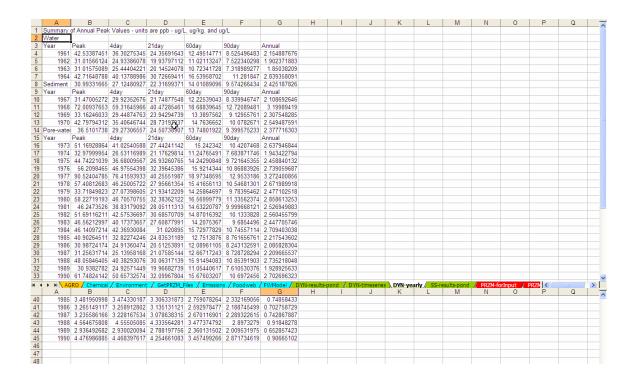


The following table summarizes the columns in the columns of the **DYN-timeseries tab:**

Table 6: Summary of timeseries output parameters included with the model

Variable/Parameter	Description (if necessary)
Time (h)	
Year	From PRZM3.12
Month	From PRZM3.12
Day	From PRZM3.12
Emission kg/year	(if it occurs at this output interval)
Fugacity, Pa	
Water	
Sediment	
Inflow	
Air	
Pure Phase Chemical	
Bulk Concentrations (natural units)	
Water, ng/L	
Sediment, ng/m3	
Inflow, ng/L	
Air, ug/m3	
Foodweb Concentrations, ng/g	
Water-dissolved only, ug/L	
Sediment-solids only	
Phytoplankton	
Zooplankton	
Benthic Invertebrates	
Forage Fish A	
Forage Fish B	
Piscivorous Fish	
Other	
SumInput kg	Cumulative system Input of chemical
SumLoss kg	Cumulative system Loss of chemical
Water inflow m3/h	
Water outflow m3/h	
Net water m3/h	Inflow-Outflow
Sed Inflow m3/h	
Sed Resusp m3/h	
Sed outflow m3/h	
Sed Dep m3/h	
Net Sed m3/h	Inflow + Resusp – Outflow – Dep

The **DYN-yearly** tab contains the Estimated Environmental Concentrations (EECs) for the peak, 4-day, 21-day, 60-day, 90-day and Annual running averages for the chemical dissolved water column (for the highest 4 years of the simulation), benthic sediment sorbed chemical (for the highest 4 years of the simulation), and chemical dissolved in benthic pore water (for all years).

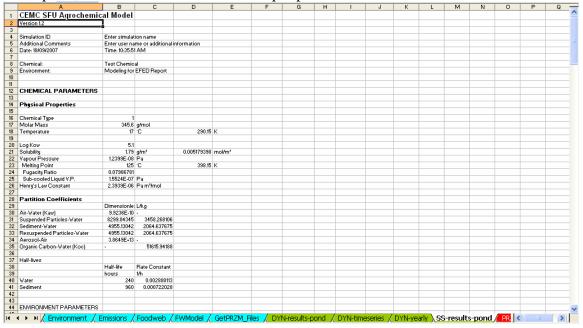


Steady-state Results

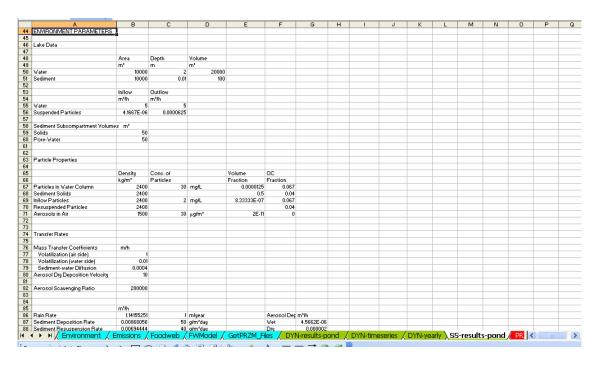
The results presented in the **SS-results-pond** tab are in the same format as the QWASI model with the foodweb results output at the bottom.

The following series of pages display an example of output contained in the **SS-results-pond** tab.

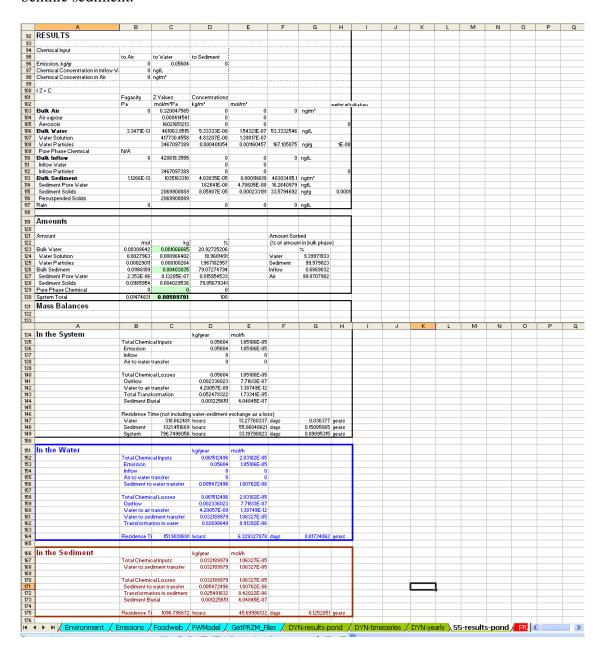
SS-results-pond tab, Rows 1 - 44 display the model version number, scenario descriptors, and echoes of the chemical input parameters.



SS-results-pond tab, Rows 44 - 88 display echoes of the environment input parameters.



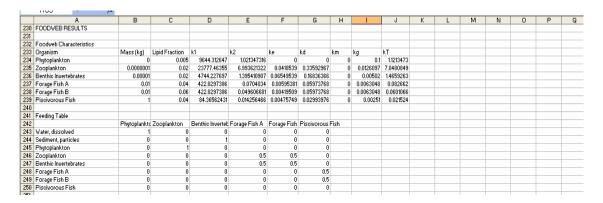
SS-results-pond tab, Rows 92 - 228 display results from the QWASI water quality model. These include mass balances for the chemical in both water and benthic sediment.



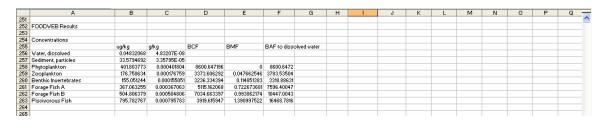
SS-results-pond tab, Rows 92 - 228, continued.

Name Box A	В	С	D	E	F	G	Н	L	J	K	L	М	N	0	Р	Q
178 Hate Details																
179																
180	kg/year	mol/h														
181 Emission to Water	0.05604															
182 Water Inflow	0.00001								_							
183 Particle Inflow	0															
184					-				_			_		-		
	-							_	-							-
185 Rain Dissolution																
186 Aerosol Deposition - Wet	0															
187 Aerosol Deposition - Dry	0	0														-
188																
189 Absorption	0															
190 Volatilization	4.2006E-09	1.38749E-12														
191																
192 Sediment Deposition	0.03049682	1.00734E-05														
193 Sediment Resuspension	0.0049026	1.61938E-06														
194																
195 Water to Sediment Diffusion	0.00169316	5.59267E-07														
196 Sediment to Water Diffusion	0.00056989															
197	0.0000000															
198 Water Transformation	0.02698649	8.91392E-06														
199 Sediment Transformation	0.02536643				-	-			_	_						
200	0.02043103	0.42U22E-U0							_							
	0.00400505	4040455.00														_
201 Sediment Burial	0.00122565	4.04845E-07														
202																-
203 Water Outflow	0.00211645															
204 Particle Outflow	0.00021958	7.25286E-08														
205																
206																1
207 D Values & Response Time	-				-											
208 D Values & nesponse Time	5								_							
209	D. W. L.	D T'-			D 7					_		_				_
209	D Value	Response Time			Response T											
210		of Water			of Sediment											-
211	mol/Pa.h	years	days	hours	years	days	hours									
212 Burial	3593591.82				3.28833472											
213 Sediment Transformation	74741721.8	0	0	0	0.15810357	57.7078016	1385									
214 Sediment Resuspension	14374367.3	0.073231566	26.72952151	641.5085163	0.82208368	300.060543	7201.5									
215 Water to Sediment Diffusion	1670921.82	0.629986041	229.9449048	5518.677716	7.07210391	2581.31793	61952									
216 Sediment Deposition	30096331.5	0.03497627	12.76633863	306.3921272	0.39263698	143,312498	3439.5									
217 Water Transformation	26632098.2			346,2468098			0									
218 Volatilization	4.14540877			2224455908												
219 Volat. (air side)	4.14540918		52555002.05	EEE 1100000					_	_						
220 Volat. (water side)	41773045.6								_							
			100.0550000	4414.040470					-	_		-		-		
221 Water Outflow	2088652.28			4414.942173												
222 Water Particle Outflow	216693.587			42554.46211					-			-		-		
223 Rain Dissolution	476861.251			19337.44672												-
224 Wet Particle Deposition	73158.2247			126045.6916												
225 Dry Particle Deposition	32043.3024			287775.5516												
226 Water Inflow	2088652.28	0.503988833	183.9559239	4414.942173												
227 Water Particle Inflow	14446.2391	72.86722964	26596.53882	638316.9317												
228																

SS-results-pond tab, Rows 230 - 250 display echoes of the input for the Food Web aquatic organism masses, lip fraction, k-rates and feeding table matrix used by the Bioaccumulation model.



SS-results-pond tab, Rows 251 - 263 display calculated results of pesticide concentrations from the Bioaccumulation model for each aquatic organism in the food web. Bioconcentration Factors (BCFs), Biomagnification Factors (BMFs) and Bioaccumulation Factors (BAFs) are presented here.



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